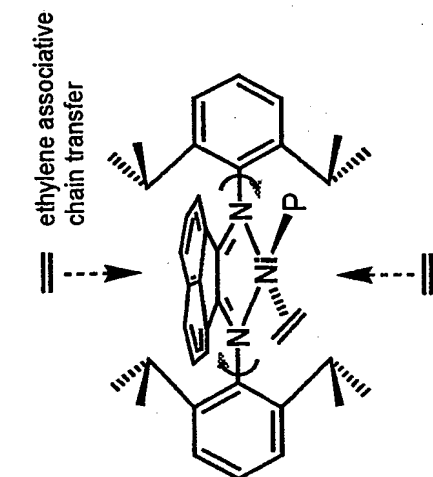
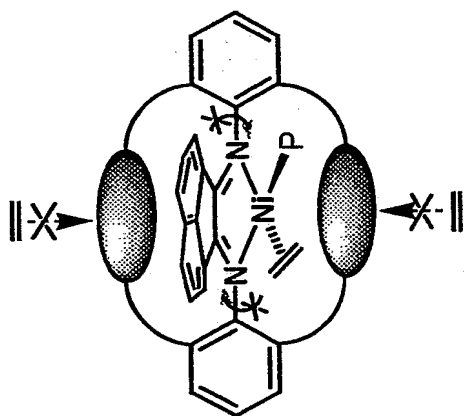


1/16

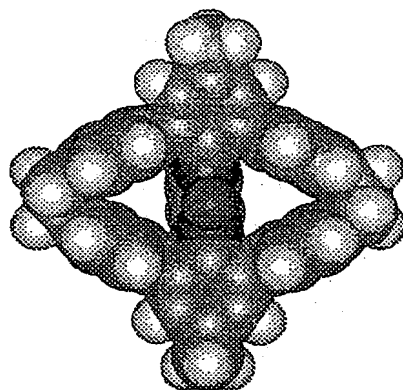
FIG. 1



A. Acyclic α -diimine complex
(catalyst **4g** in reference 5)



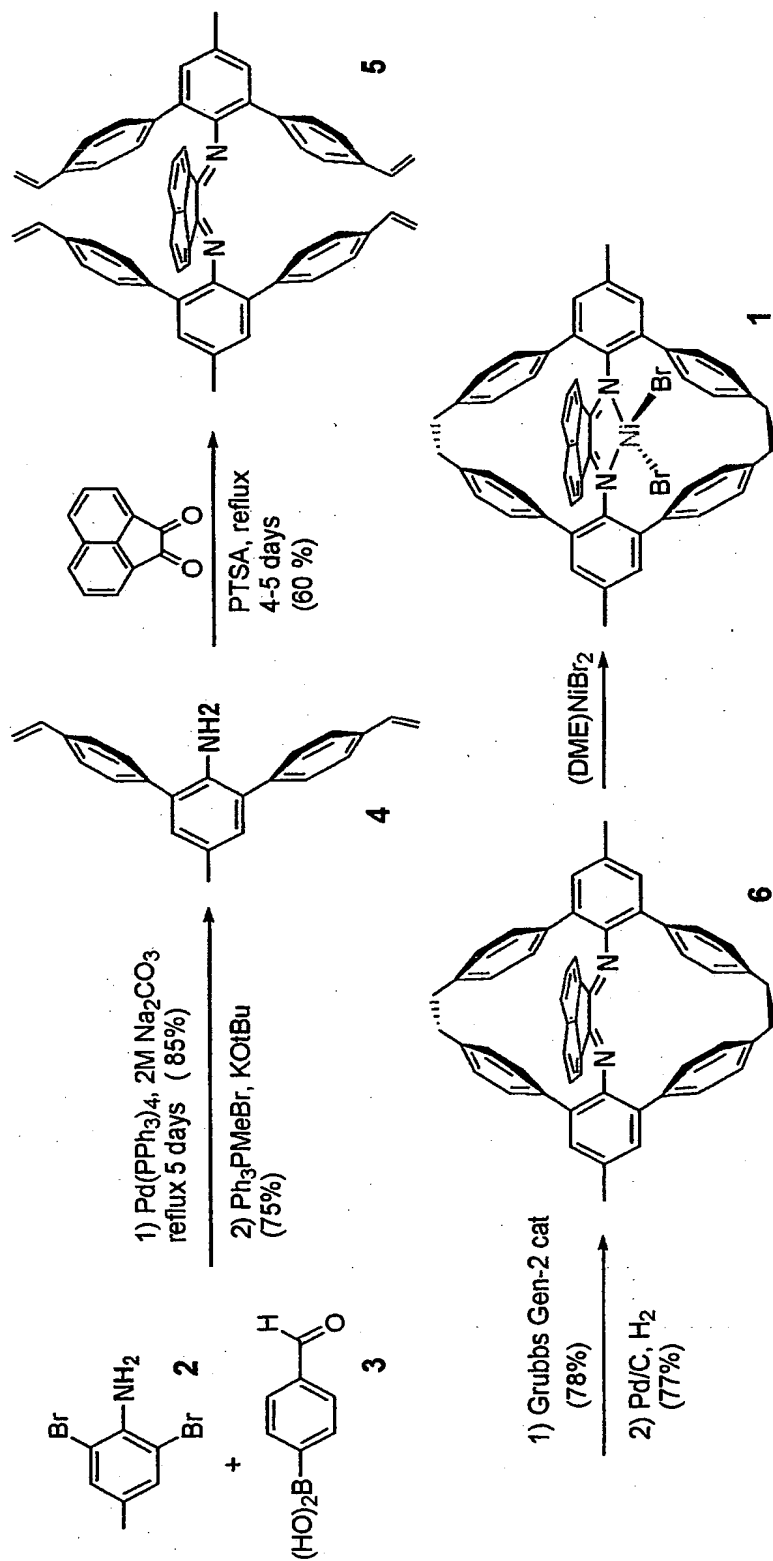
B. Cyclophane-based
 α -diimine complex



C. Molecular model of
complex **1**

2/16

FIG. 2



3/16

FIG. 3

Summary of Polymerization Data

Entry	Moles of Catalyst ($\times 10^{-3}$)	Temp. (°C)	Time (min)	Yield (g)	TON ^b ($\times 10^{-3}$)	TOF ^b ($\times 10^{-3}$ /h)	M_n ^b ($\times 10^{-3}$)	M_w ^b ($\times 10^{-3}$)	PDI	Branches Per 1000 carbons
1	1	30	5	3.48	124	1 491	320	413	1.29	66
2	1	30	10	6.70	239	1 436	288	374	1.30	73
3	1	30	15	9.25	331	1 321	294	386	1.31	67
4	1	50	5	3.20	114	1 371	248	305	1.23	80
5	1	50	10	6.85	245	1 468	652	834	1.28	84
6	1	50	15	9.00	321	1 286	342	422	1.23	85
7	1	70	5	3.11	111	1 333	323	468	1.45	91
8	1	70	10	6.10	218	1 307	619	886	1.43	89
9	1	70	15	7.35	263	1 050	429	605	1.41	91
10	1	90	5	2.50	89	1 071	252	433	1.72	97
11	1	90	10	4.70	168	1 007	462	756	1.64	96

^a Experimental condition: in 200 mL of toluene, cocatalyst MMAO (Al:Ni \approx 3000), 200 psi ethylene pressure.^b TON = turnover number, which was calculated as the moles of ethylene per mole of catalyst; TOF = turnover frequency, i.e., TON per hour.

FIG. 4A

Examples of bidentate ligands

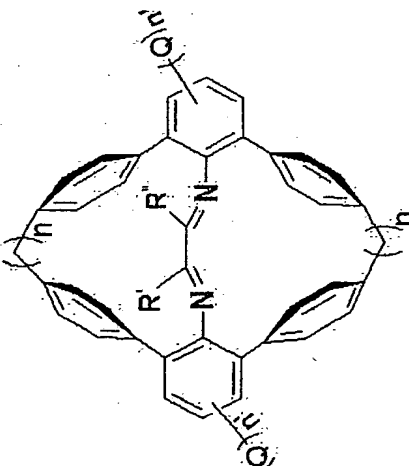
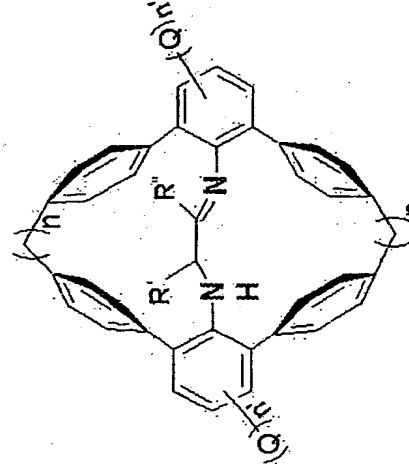
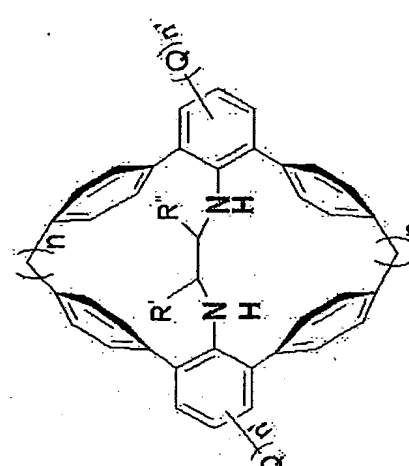
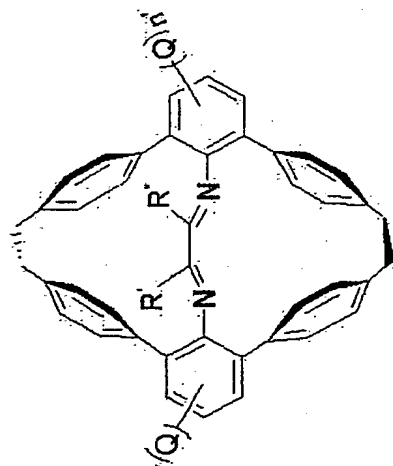
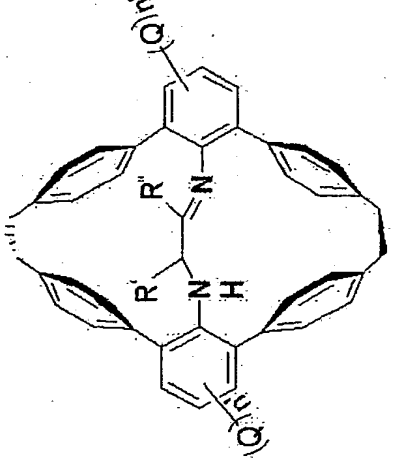
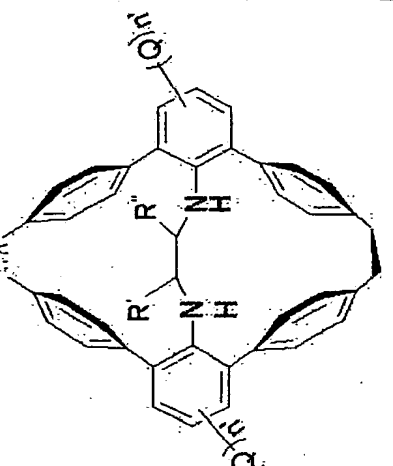
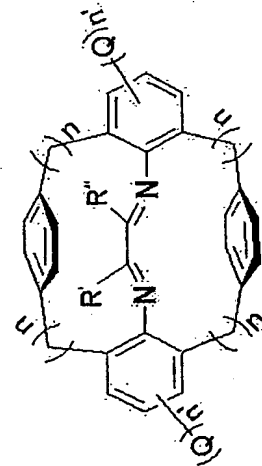
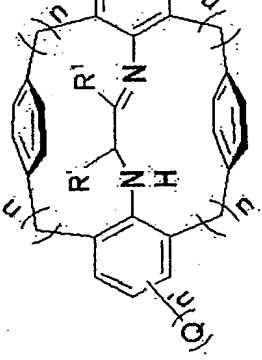
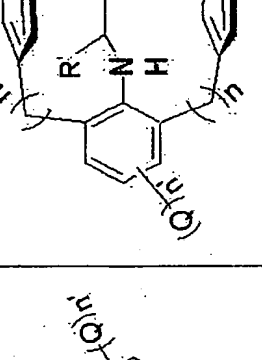
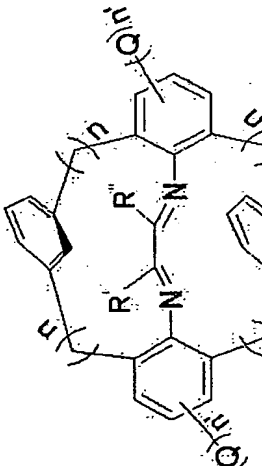
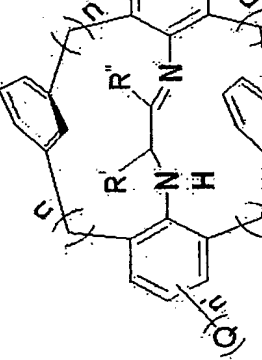
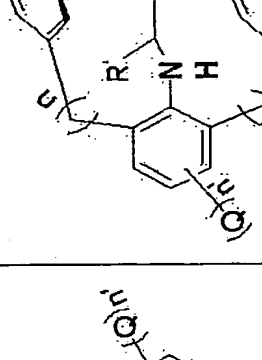
$B_1 = B_2 = -Ar-T-Ar-$ 	$B_1 = B_2 = -Ar-T-Ar-$ 	$B_1 = B_2 = -Ar-T-Ar-$ 
1. $B_1 = B_2 = -Ar-T-Ar-$ 	2. $B_1 = B_2 = -Ar-T-Ar-$ 	3. $B_1 = B_2 = -Ar-T-Ar-$ 
4.	5.	6.

FIG. 4B

Examples of bidentate ligands (continued)

FIG. 4C

Examples of bidentate ligands (continued)

$B_1 = B_2 = -T-Ar-T-$ 	$B_1 = B_2 = -T-Ar-T-$ 	$B_1 = B_2 = -T-Ar-T-$ 
$B_1 = B_2 = -T-Ar-T-$ 	$B_1 = B_2 = -T-Ar-T-$ 	$B_1 = B_2 = -T-Ar-T-$ 

7/16

FIG. 4D

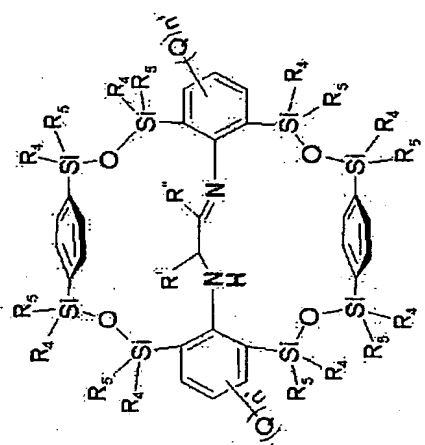
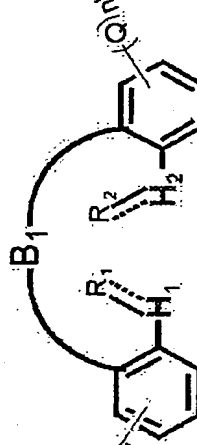
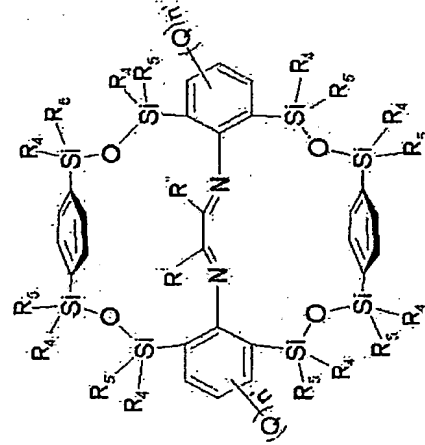
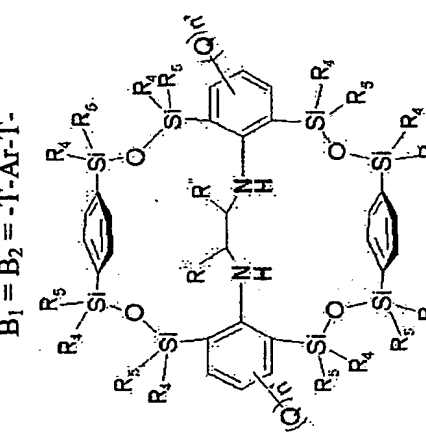
Examples of bidentate ligands (continued)

$B_1 = B_2 = -T-Ar-T-$	$B_1 = B_2 = -T-Ar-T-$	$B_1 = B_2 = -T-Ar-T-$
19.	20.	21.
$B_1 = B_2 = -T-Ar-T-$	$B_1 = B_2 = -T-Ar-T-$	$B_1 = B_2 = -T-Ar-T-$
22.	23.	24.

8/16

FIG. 4E

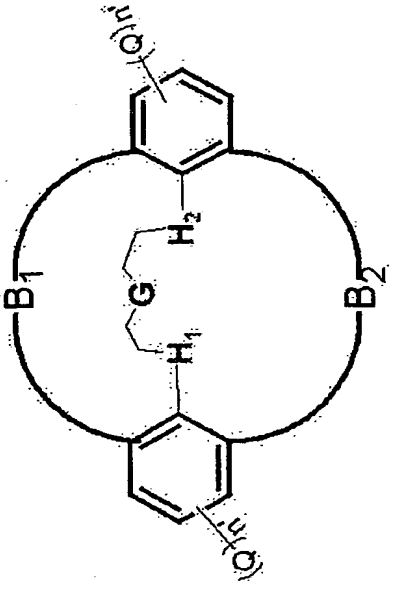
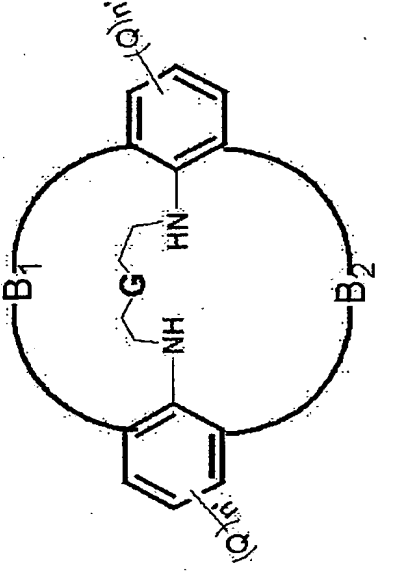
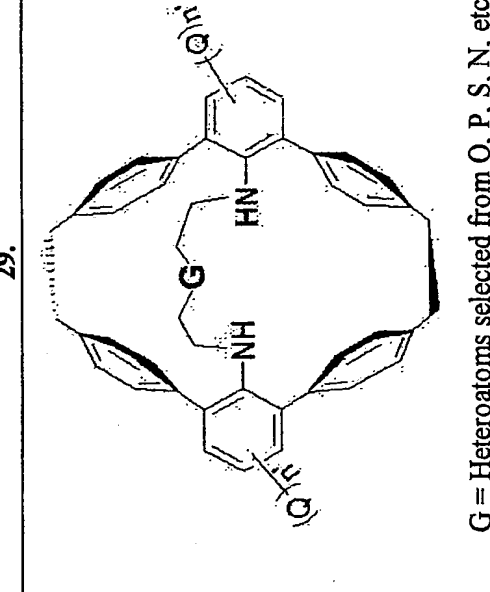
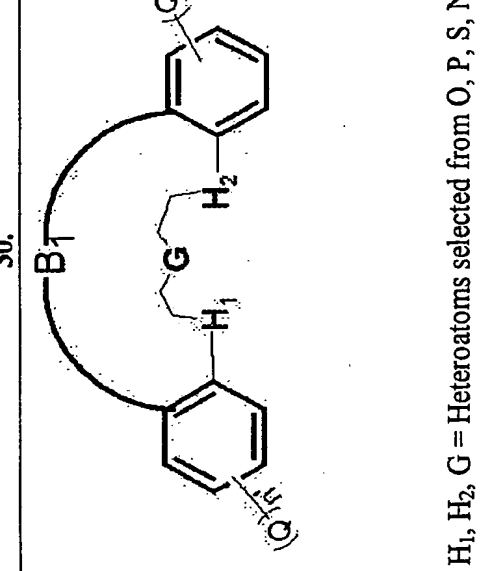
Examples of bidentate ligands (continued)

<p>$B_1 = B_2 = -T-Ar-T-$</p> 	<p>25.</p> <p>$B_1 = B_2 = -T-Ar-T-$</p>  <p>half-cyclic structure for any of the above ligands</p>
<p>$B_1 = B_2 = -T-Ar-T-$</p> 	<p>27.</p> <p>$B_1 = B_2 = -T-Ar-T-$</p> 

9/16

FIG. 5A

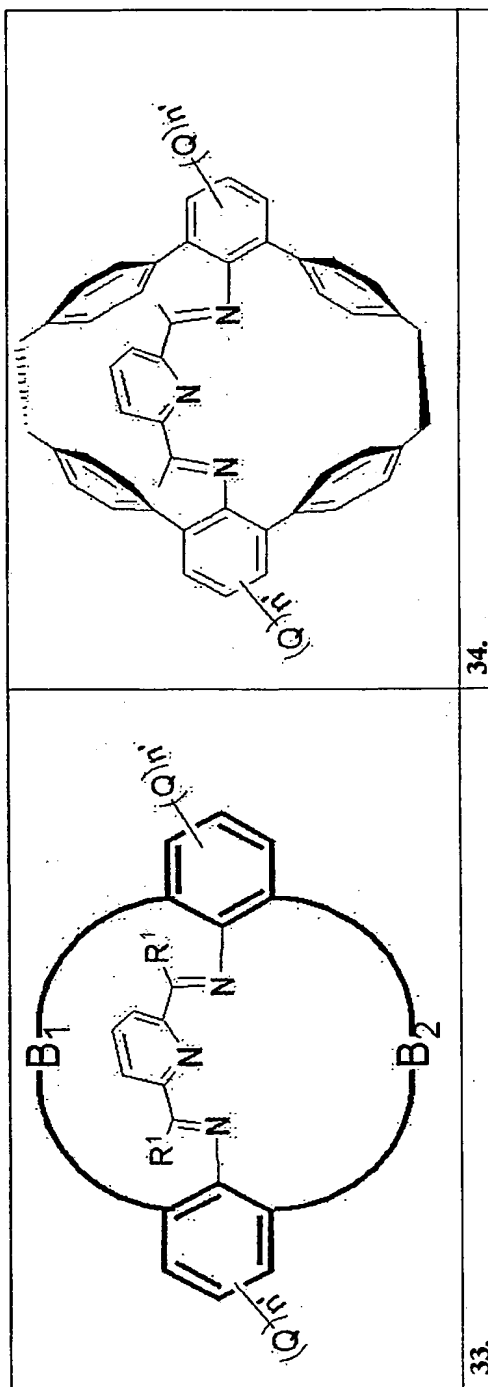
Examples of tridentate ligands

 <p>H₁, H₂, G = Heteroatoms selected from O, P, S, N, etc.</p>	 <p>G = Heteroatoms selected from O, P, S, N, etc.</p>
 <p>G = Heteroatoms selected from O, P, S, N, etc.</p>	 <p>H₁, H₂, G = Heteroatoms selected from O, P, S, N, etc.</p>

10/16

FIG. 5B

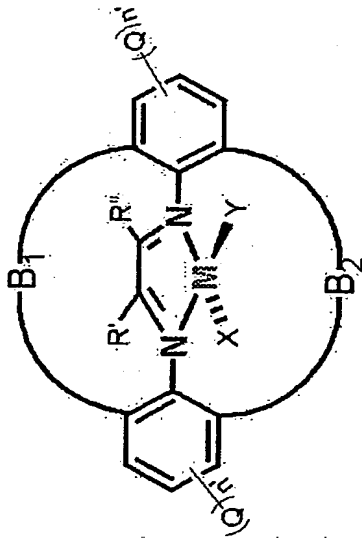
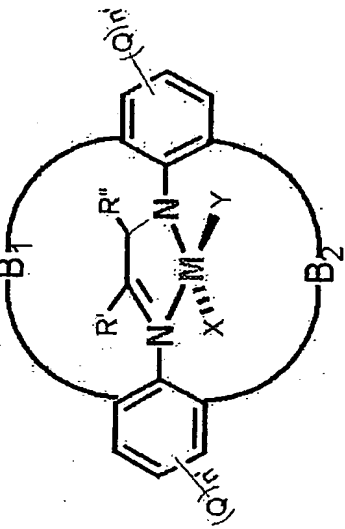
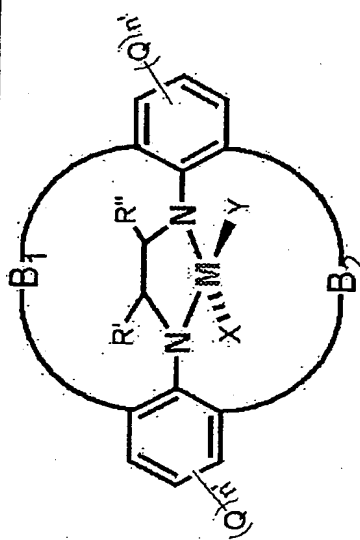
Examples of tridentate ligands (continued)



11/16

FIG. 6A

Examples of preference of metals for different types of ligands

 <p>For this type of ligand, preferred M are late transition metals such as Fe, Ru, Os, Rh, Ir, Ni, Pd, Pt, Cu, and most preferred are Ni and Pd.</p>	 <p>For this type of ligand, preferred M are Zn and Al.</p>
 <p>For this type of ligand, preferred M are early transition metals such as Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and W, and most preferred are Ti, Zr, Hf, V, and Cr.</p>	<p>36</p>
<p>35</p>	<p>37</p>

12/16

FIG. 6B

Examples of preference of metals for different types of ligands (continued)

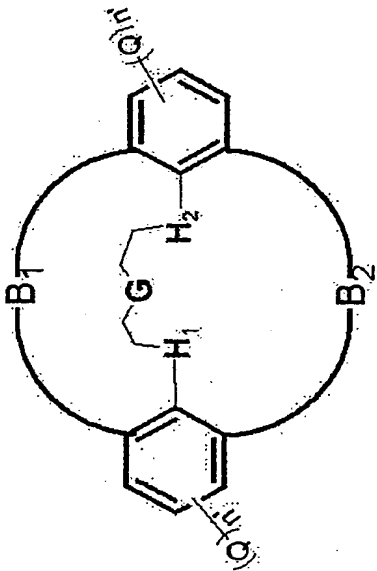
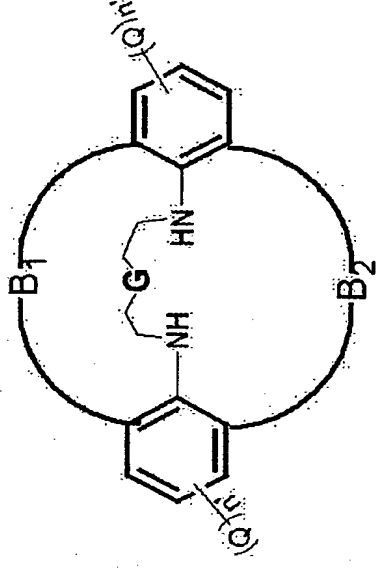
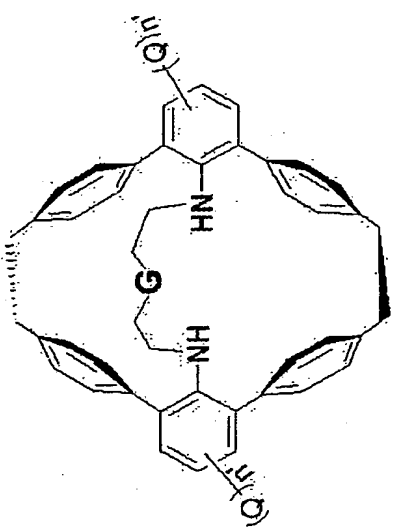
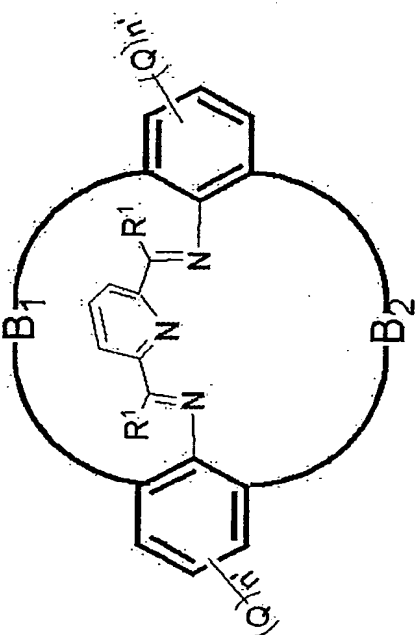
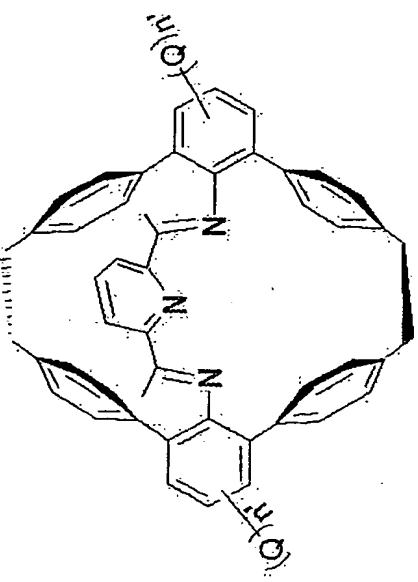
 <p>$H_1, H_2, G = \text{Heteroatoms selected from O, P, S, N, etc.}$</p>	 <p>$G = \text{Heteroatoms selected from O, P, S, N, etc.}$</p>
<p>38.</p>  <p>40.</p>	<p>39.</p> <p>For this type of ligand, preferred M are early transition metals such as Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and W, and most preferred are Ti, Zr, Hf, V, and Cr; G = Heteroatoms selected from O, P, S, N, etc.</p>

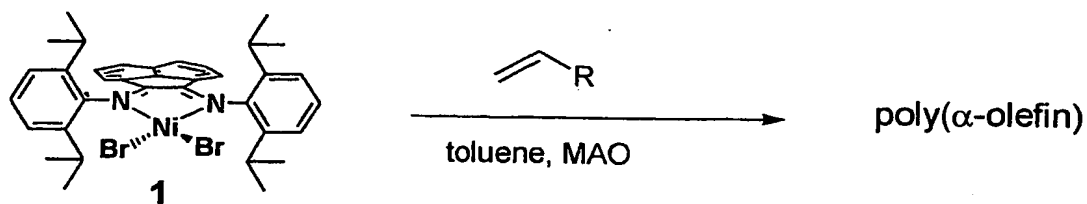
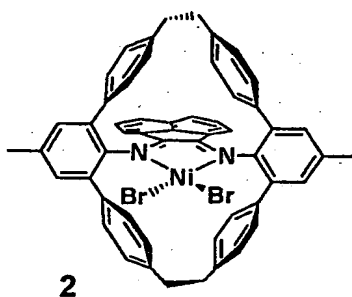
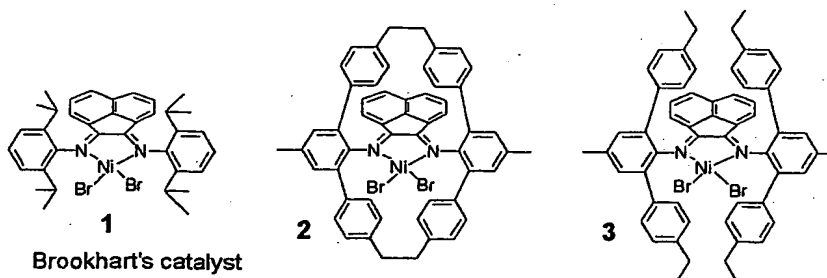
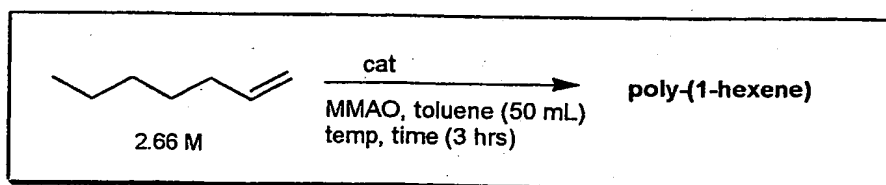
FIG. 6C

Examples of preference of metals for different types of ligands (continued)

	
For this type of ligand, most preferred M are Fe and Co.	
41.	42.

In structures 1 through 42, Q, n, R₄ and R₅ are as defined in Formula 1 in the specification, n' is 1 through 4, and R' and R'' are alkyl, alkenyl, aryl, aralkyl, or cycloalkyl.

14/16

FIG. 7
(Prior Art)**FIG. 8****FIG. 9**

15/16

FIG. 10

Polymerization of 1-Hexene
(Catalyst Activity and Molecular Weight Data at 0 °C and at 25 °C)

entry	c at	Load (mmol)	Temp (°C)	Yield (g)	TON	Mw	Mn	PDI	DSC (°C)	Branch /1000c
F62	2	0.005	0	0.33	784	170 K	96 K	1.77	T _m 58	65
F36	2	0.01	0	0.41	488	305 K	292 K	1.05	T _m 63	61
F84	1	0.005	0	1.62	3850	719 K	627 K	1.15	T _m -42	104
Ref JACS 95, 6414	1	0.017 activated by Et ₂ AlCl	0	2.1	1468	310 K	140 K	2.2	T _m -20 T _g -57	100
F60	2	0.005	25	1.68	3992	623 K	510 K	1.22	T _m 62	57
F72	1	0.005	25	1.90	4515	817 K	543 K	1.50	T _m -50	108
Ref JACS 96, 11664	1	0.017 3.2 M; 30 min rxn.	23	---	2800	129 K	84 K	1.54	T _m -17 T _g -57	120
F74	3	0.005	25	0.80	1901	88 K	83 K	1.06	T _m 56	35
F42	2	0.005	75	2.21	5466	622 K	529 K	1.17	T _m 59	52
F68	1	0.005	75	0.43	1022	415 K	279 K	1.49	T _m -53	111
F70	3	0.005	75	0.26	618	131 K	92 K	1.43	T _m 73	38
F46	2	0.005	95	1.6	3802	252 K	125 K	2.00	T _m 57	54
F48	1	0.005	95	0.47	1117	287 K	171 K	1.68	T _m -53	113
F50	3	0.005	95	0.59	1402	77 K	59 K	1.29	T _m 76	40

16/16

FIG. 11